

What is claimed is:

1. A method of estimating a pure spectrum and a concentration of each component constituting  $n$  sample mixtures, in which  $p$  kinds of components are mixed, the method comprising:

(a) performing a principal component analysis of the spectra of the  $n$  mixtures, which are measured using  $m$  wavelengths, to represent the spectra of the  $n$  mixtures as factors and scores of the respective factors, wherein  $n$ ,  $p$ , and  $m$  are integers and  $m > p$ ; and

(b) performing an independent component analysis of the scores obtained in (a) to estimate the pure spectra and the concentrations of the respective components.

2. The method as claimed in claim 1, wherein the number of factors to be used is decided from among the factors obtained in (a) and the independent component analysis is applied to the scores of the decided factors.

3. The method as claimed in claim 1, wherein the concentrations of the components constituting the mixture are statistically independent.

4. The method as claimed in claim 2, wherein the concentrations of the components constituting the mixture are statistically independent.

5. The method as claimed in claim 1, wherein (b) comprises:

(b1) performing the independent component analysis of the scores of the factors to decompose the scores into a mixing matrix and independent components;

(b2) estimating the product of the factors obtained in (a) and the mixing matrix obtained in (b1) as the pure spectra of the respective components; and

(b3) estimating the independent components obtained in step (b1) as being proportional to the concentrations of the components contained in the mixture.

6. The method as claimed in claim 1, wherein (b) comprises:

(b1) deciding the number of the factors to be used from among the factors obtained in (a);

(b2) performing the independent component analysis of the scores of the decided factors to decompose the scores into a mixing matrix and independent components;

(b3) estimating the product of the decided factor and the mixing matrix obtained in (b2) as the pure spectrum of each component; and

(b4) estimating the independent components obtained in (b2) as being proportional to the concentrations of the components contained in the mixture.

7. The method as claimed in claim 1, wherein the ICA may be performed using a technique selected from the group consisting of: maximization of non-gaussianity (MN), maximum likelihood estimation (MLE), and minimization of mutual information (MMI).

8. The method as claimed in claim 1, wherein in (a), a low-noise band including information on a component to be estimated is decided as an analysis band from among the spectra of the  $n$  mixtures measured using  $m$  wavelengths.

9. The method as claimed in claim 1, wherein (a) comprises: performing a preprocessing step to remove scattering and noise, before performing the principal component analysis of the spectra of the  $n$  mixtures measured using  $m$  wavelengths.

10. The method as claimed in claim 9, wherein the preprocessing step comprises a technique selected from the group consisting of multiplicative scatter correction (MSC), mean-centering, and autoscaling.

11. A computer-readable medium having embodied thereon:  
  
a first program for performing a principal component analysis of a spectra of the  $n$  mixtures measured using  $m$  wavelengths to represent the spectra as factors and scores of the respective factors, wherein  $n$  and  $m$  are integers; and

a second program for performing an independent component analysis of the scores produced by the first program to decompose the scores into a mixing matrix and independent components, estimating that the product of the factor obtained by the first program and the mixing matrix is the pure spectra of each component, and estimating that the independent components are proportional to the concentrations of the components contained in the mixture.

12. The medium as claimed in claim 11, wherein the concentrations of the components constituting the mixture are statistically independent.

13. An apparatus of estimating a pure spectrum and a concentration of each component constituting  $n$  sample mixtures, in which  $p$  kinds of components are mixed, the apparatus comprising:

a principal component analysis unit for performing a principal component analysis of the spectra of the  $n$  mixtures, which are measured using  $m$  wavelengths, to represent the spectra of the  $n$  mixtures as factors and scores of the respective factors, where  $n$ ,  $m$ , and  $p$  are integers and  $m > p$ ;

an independent component analysis unit for performing an independent component analysis of the scores provided from the principal

component analysis unit, to decompose the scores into a mixing matrix and independent components;

a pure spectrum estimating unit for estimating the product of the factor provided from the principal component analysis unit and the mixing matrix as the pure spectra of each component; and

a concentration estimating unit for estimating the independent components as the concentrations of the components contained in the mixture.